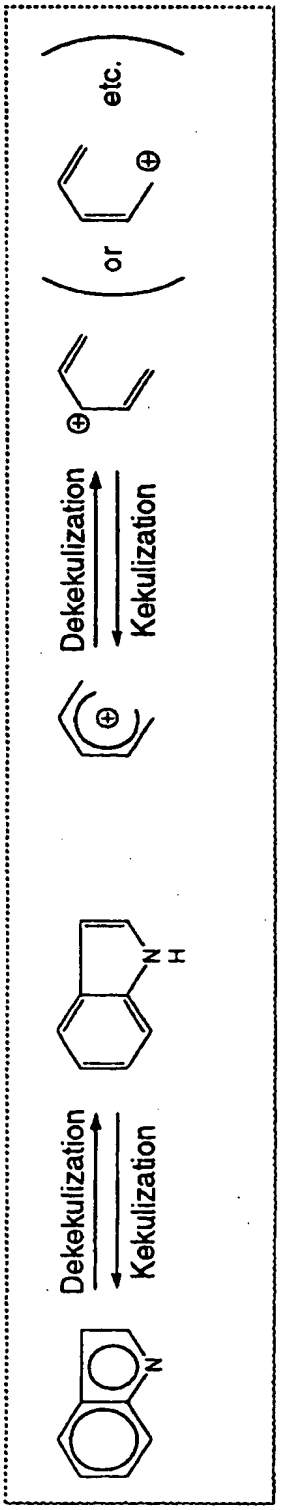

FIG. 1

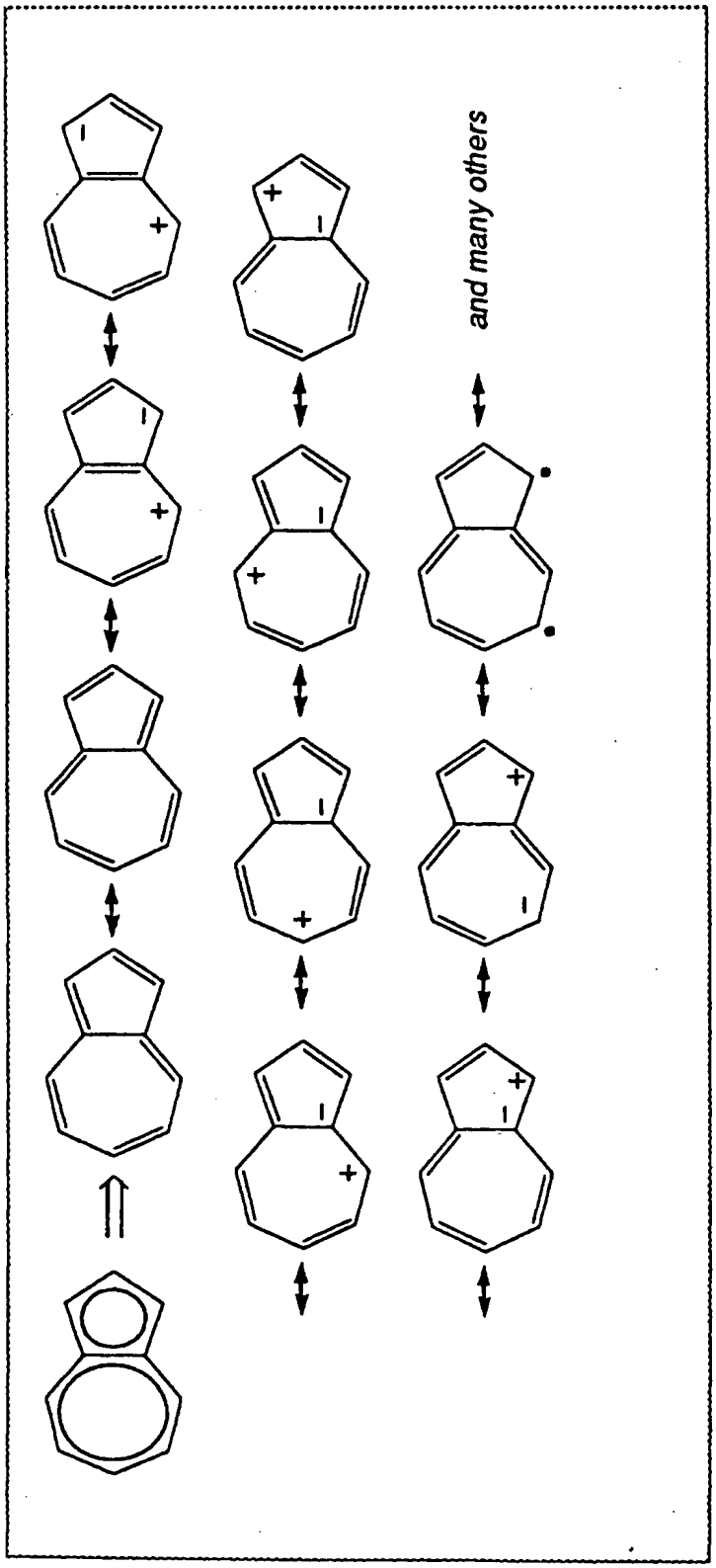

FIG. 2

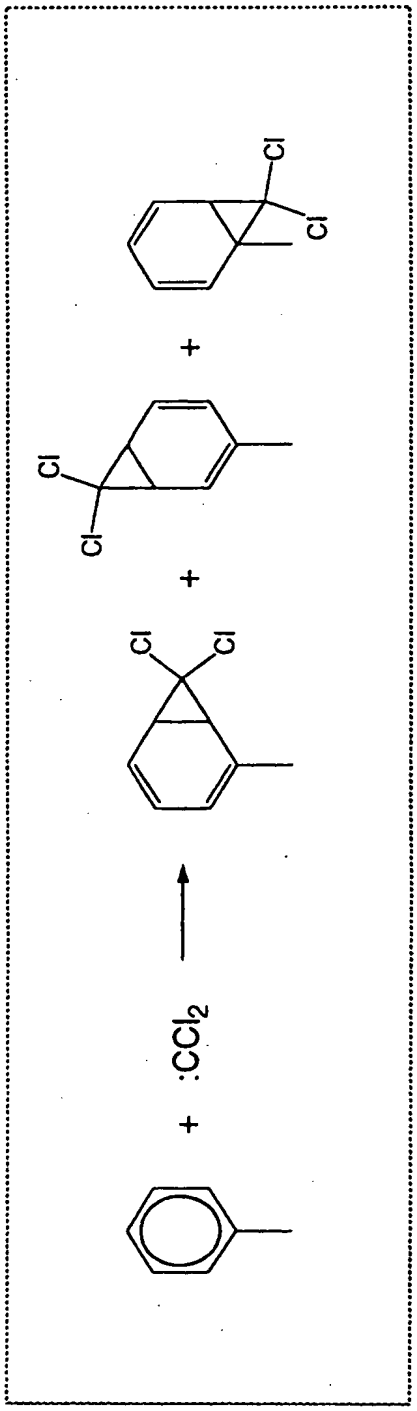

FIG. 3

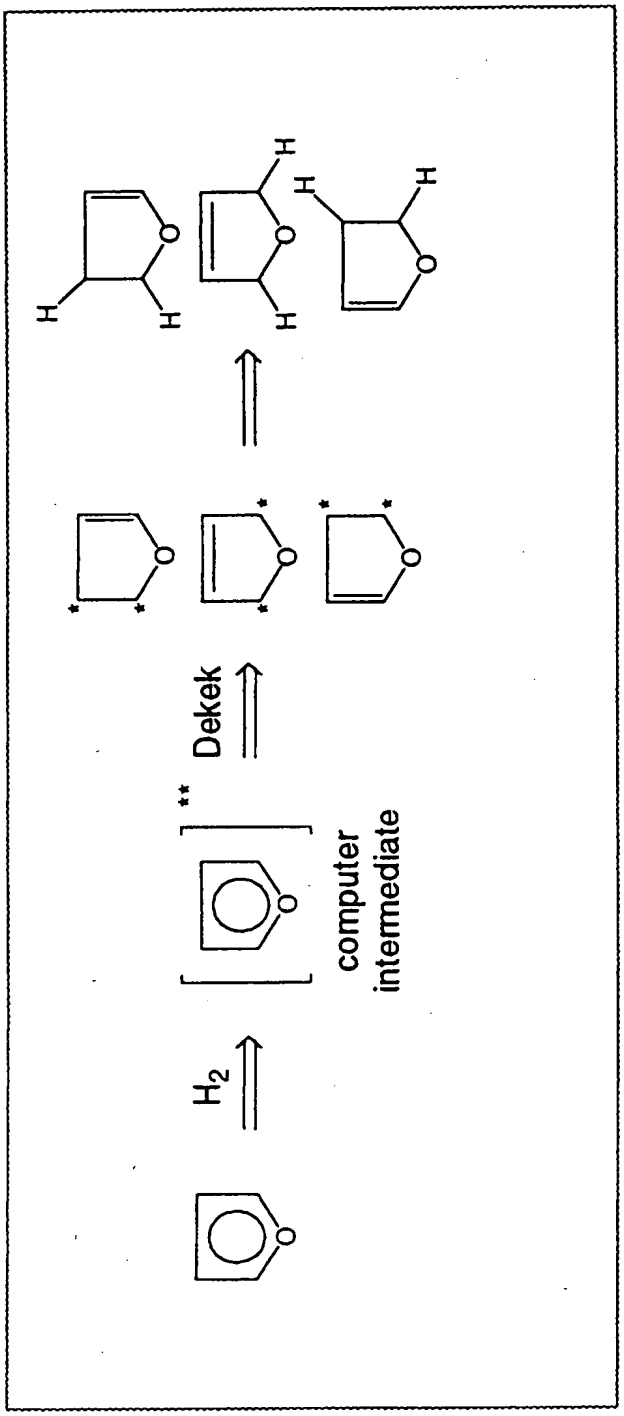

FIG. 4

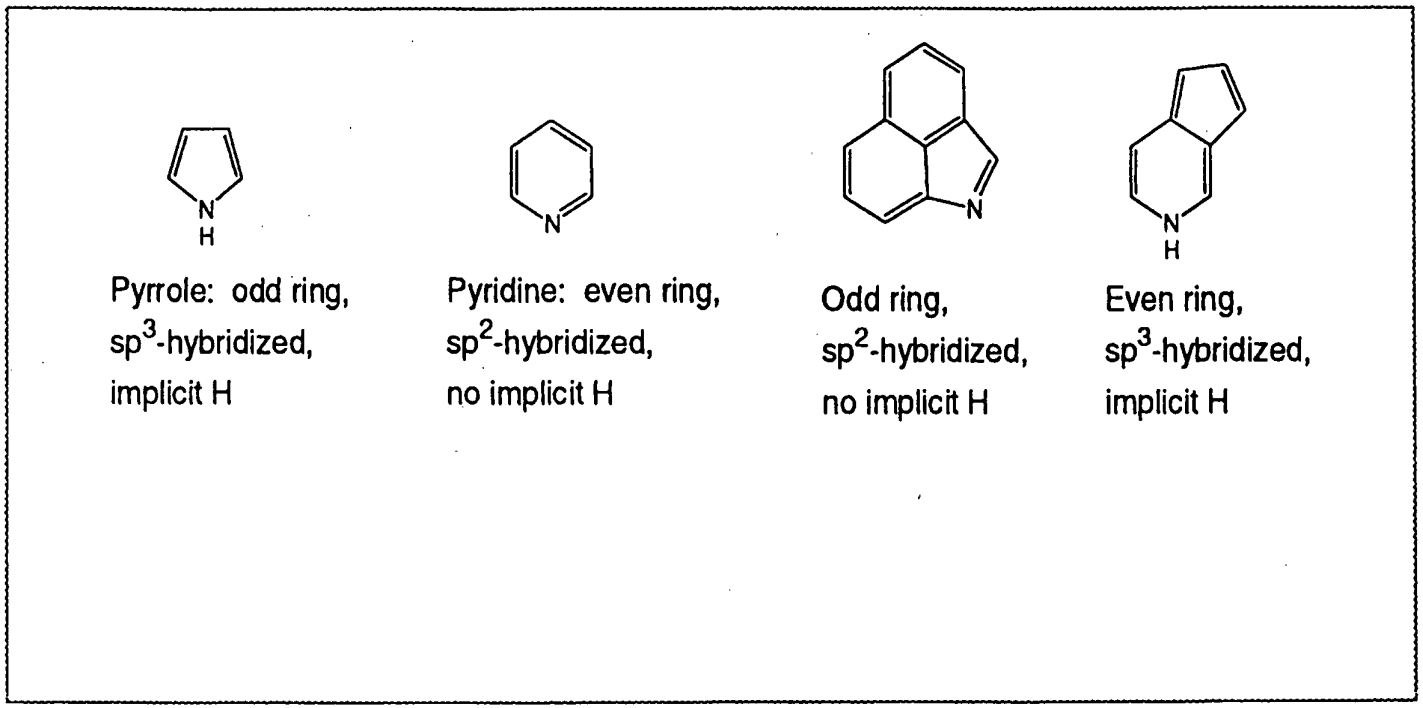

FIG. 5

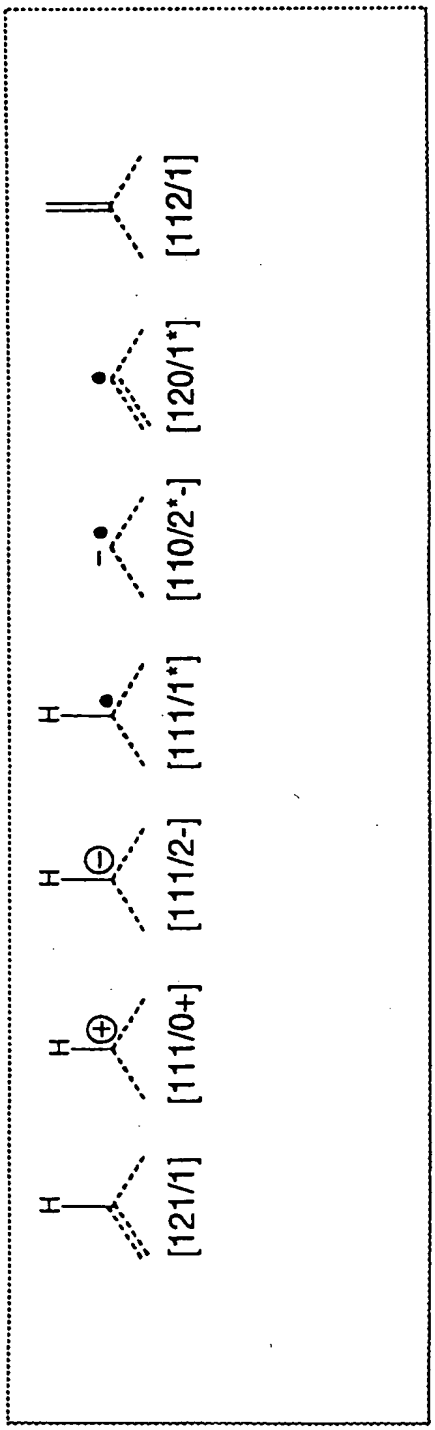

FIG. 6

Table 1. Selected Electronic State/Valence Distributions[a]

Elm	Chrg	Rad	Bd#1	Bd#2	#Extern Bds[b]	#e's Contrib	Shorthand	Structure
B			1	2	0	1	[120/1]	B-1
B			1	1	1	0	[111/0]	B-2
B	-1		1	2	1	1	[121/1-]	B-3
C			1	2	1	1	[121/1]	C-1
C	+1		1	1	1	0	[111/0+]	C-2
C	-1		1	1	1	2	[111/2-]	C-3
C		•	1	1	1	1	[111/1*]	C-4
C			1	1	2	1	[112/1]	C-5
N			1	2	0	1	[120/1]	N-1
N			1	1	1	2	[111/2]	N-2
N	+1		1	2	1	1	[121/1+]	N-3
N	+1	•	1	1	1	1	[111/1+*]	N-4
O			1	1	0	2	[110/2]	O-1
O	+1		1	1	1	2	[111/2+]	O-2
O	+1		1	2	0	1	[120/1+]	O-3
P like N[c]								
P			1	2	2	1	[122/1]	P-1
S like O								
S			2	2	0	2	[220/2]	S-1
Cl	+1		1	1	0	2	[110/2+]	Cl-1
Cl			1	2	2	1	[122/1]	Cl-2
Cl			1	2	4	1	[124/1]	Cl-3

FIG. 7

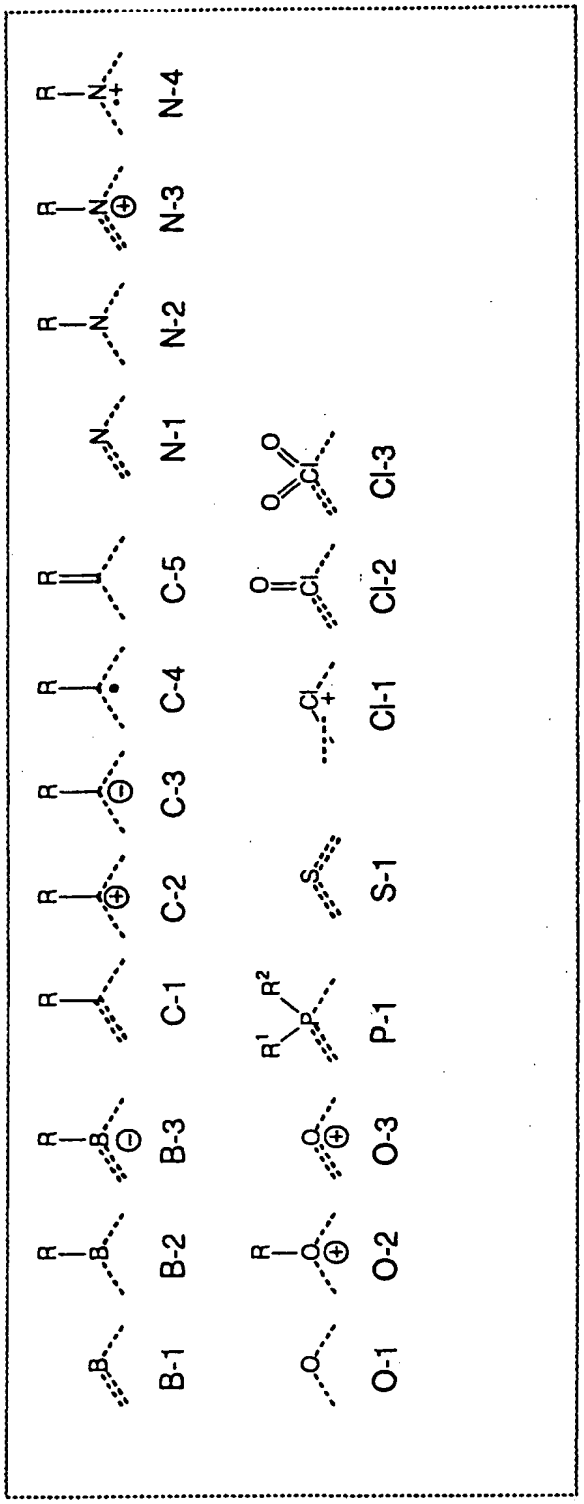

FIG. 8

Table 2. Procedure Control Flags

Flag	Meaning
kDontAssumeImpH	Otherwise, heteroatoms might carry undrawn hydrogens.
kIfFailWithOneSystem_FailWithAll	If given two or more delocalized systems and one fails, the molecule is returned unchanged, and the procedure fails.
kDoNotCreateCharges	Do not create zwitterions, i.e., more charges than necessary to achieve the system's net charge.
kDoNotCreateRadicals	Do not create more than one radical.
kConfineChargesToHeteroatoms	All charged atoms must be heteroatoms.
kConfineRadicalsToHeteroatoms	All atoms with an unpaired electron must be heteroatoms.
kFavorMultiplyBondedHetero	When a system can support more or fewer multiple bonds, favor the form with more multiple bonds (even if it is anti-aromatic).
kDisfavorAntiaromaticSystems	Use this flag in conjunction with the previous.
kSolutionMustBeFullyAlternating	Bonds must alternate as single and double.

FIG. 9

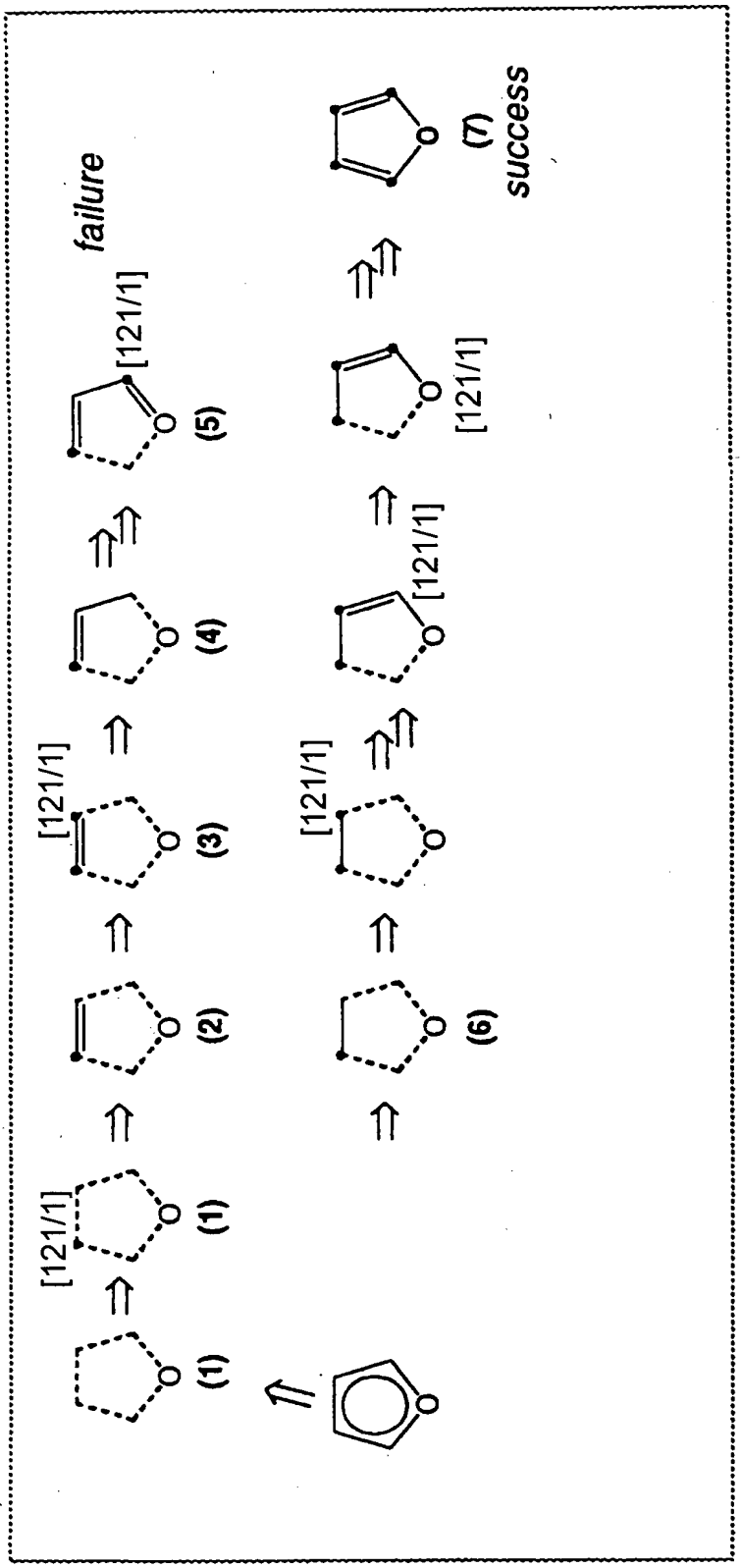

FIG. 10

Table 3. Meanings of bits in the ESVD Screening Bitmask (ESB) and Atom Screening Bitmask (ASB)

Bit #	Description	Bit #	Description
0	Has an internal single bond	8	Charge = 0
1	Has two internal single bonds	9	Charge = +1
2	Has an internal double bond	10	Charge = -1
3	Has two internal double bonds	11	Charge ≠ -1
4	Has an external bond	12	Charge ≠ +1
5	Does *not* have an external bond	13	Radical present
		14	Radical not present

FIG. 11

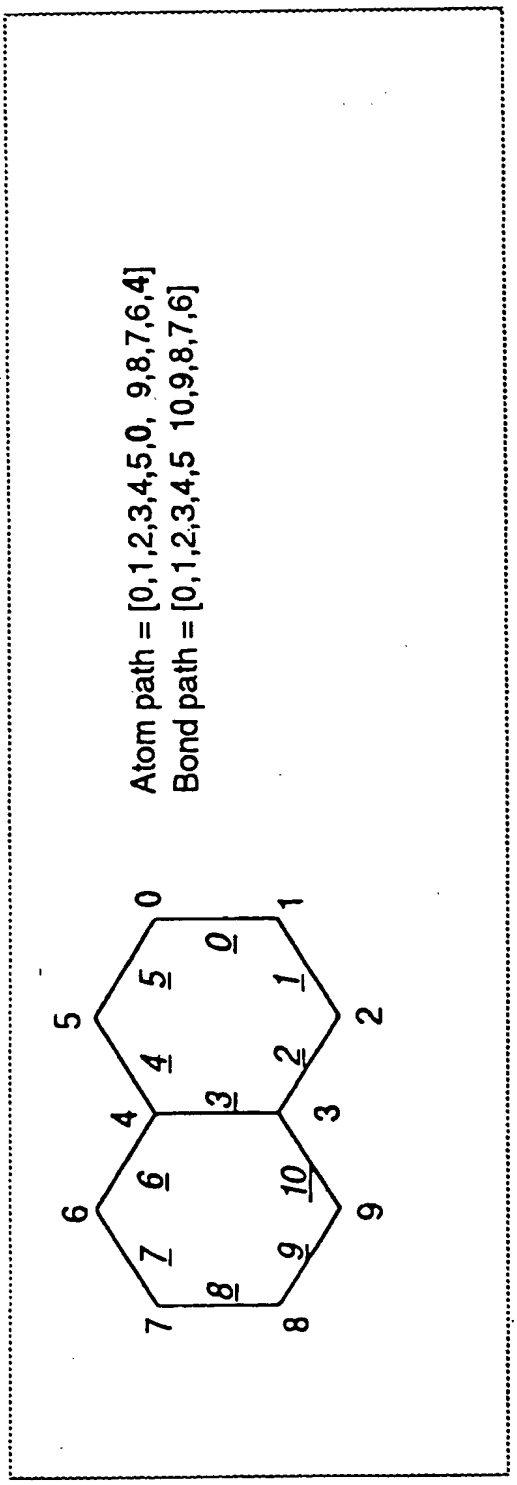

FIG. 12

Action #	Action	Atom / Bond	Action #	Action	Atom or Bond
1	Assign ESVD	Atom 0	14	Assign Bond	Bond 10
2	Assign Bond	Bond 0	15	Assign ESVD	Atom 9
3	Assign ESVD	Atom 1	16	Assign Bond	Bond 9
4	Assign Bond	Bond 1	17	Assign ESVD	Atom 8
5	Assign ESVD	Atom 2	18	Assign Bond	Bond 8
6	Assign Bond	Bond 2	19	Assign ESVD	Atom 7
7	Assign ESVD	Atom 3	20	Assign Bond	Bond 7
8	Assign Bond	Bond 3	21	Assign ESVD	Atom 6
9	Assign ESVD	Atom 4	22	Assign Bond	Bond 6
10	Assign Bond	Bond 4	23	Verify completed	Atom 4
11	Assign ESVD	Atom 5	24	Complete	---
12	Assign Bond	Bond 5			
13	Verify completed	Atom 0			

FIG. 13

Table 4. The Actions Comprising a Strategy

Action	Applies To	Explanation
Assign ESVD	Atom	Find the ESVD's for the current atom that are compatible with its environment. The best one is used directly, and if there is more than one, the rest are queued.
Assign Bond	Bond	Assign a bond order to the current bond, consistent with the ESVD of the previous atom, i.e. the (earliest occurring) atom adjacent to the bond. (The bond's other atom has not been encountered yet, unless the bond closes a ring. Even in this case, the other atom's environment is not taken into account. It will be checked in the next Action.)
Verify Completed	Atom	This Action is taken just after the last bond in a ring or acyclic chain is fixed. Ordinarily the bonds of an atom are sure to be compatible with its assigned ESVD because its ESVD was picked to be compatible with the bond leading to it, and the bond leading away from it was selected to be compatible with its ESVD. However, a ring closure atom has not had its ESVD checked with respect to the ring closure bond, nor has a terminal atom in an acyclic chain. Thus, in this Action the atom is checked to verify that its final bonding environment is compatible with its ESVD.
Complete	---	Signifies that the path is completed, and all atoms have been assigned compatible ESVD's and bond orders. If the net charge or radical count of the putative solution is wrong, the solution is rejected. If the solution is perfect, as defined elsewhere, it is returned directly and the procedure terminates. Otherwise, if it is the best solution yet, it displaces the previous best candidate.

FIG. 14

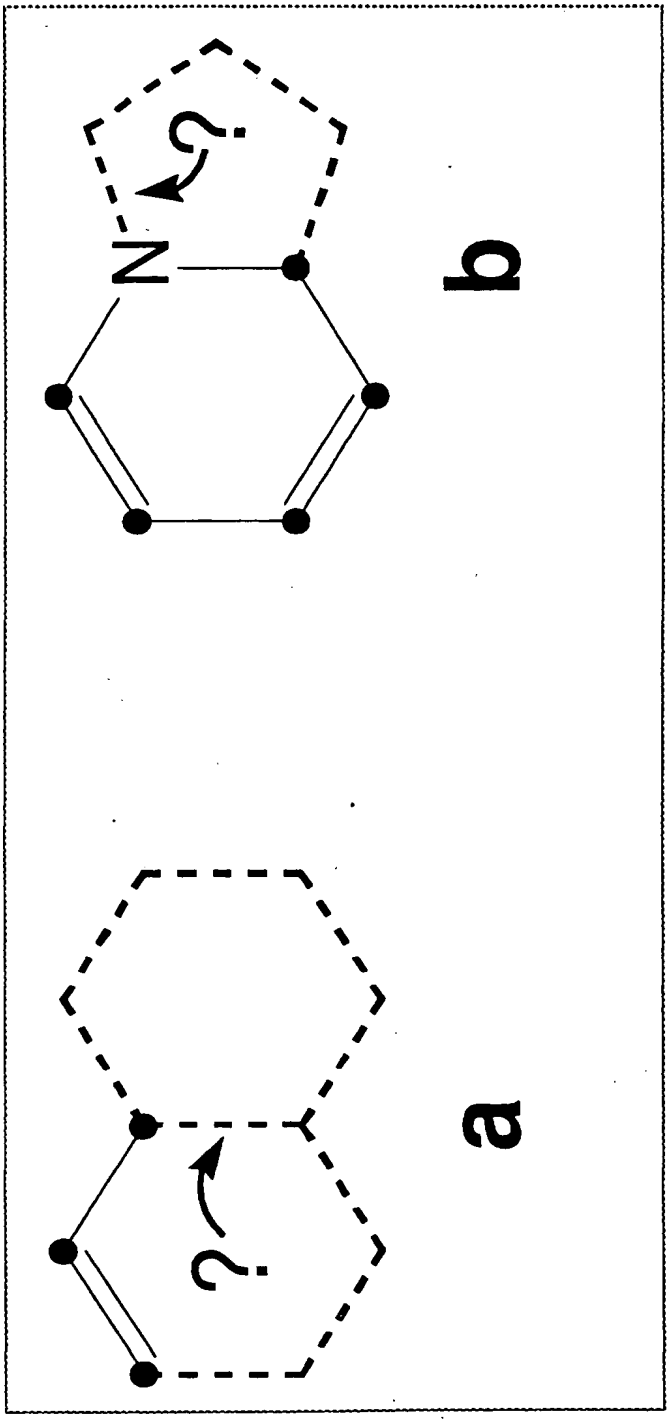

FIG. 15

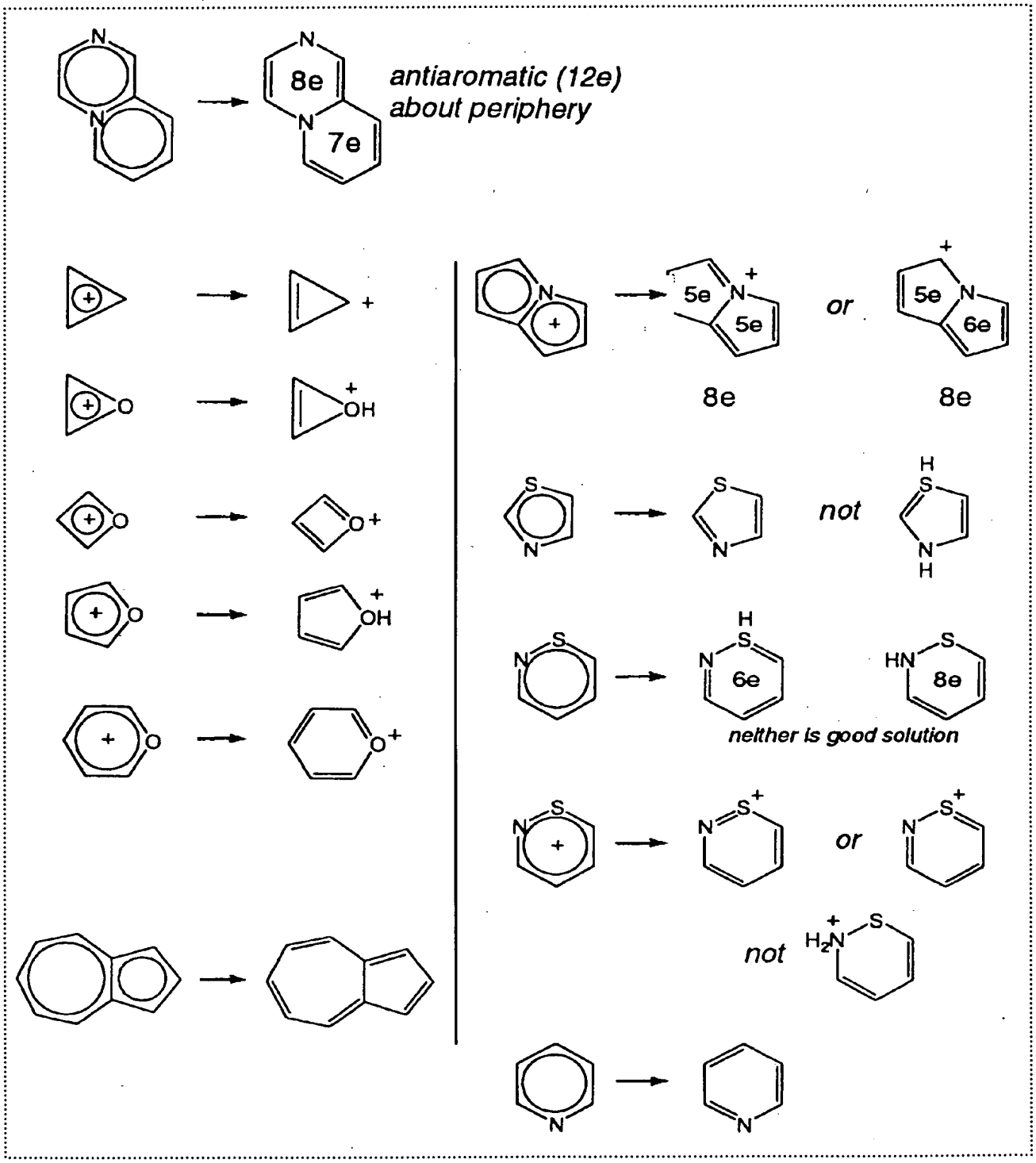

FIG. 16

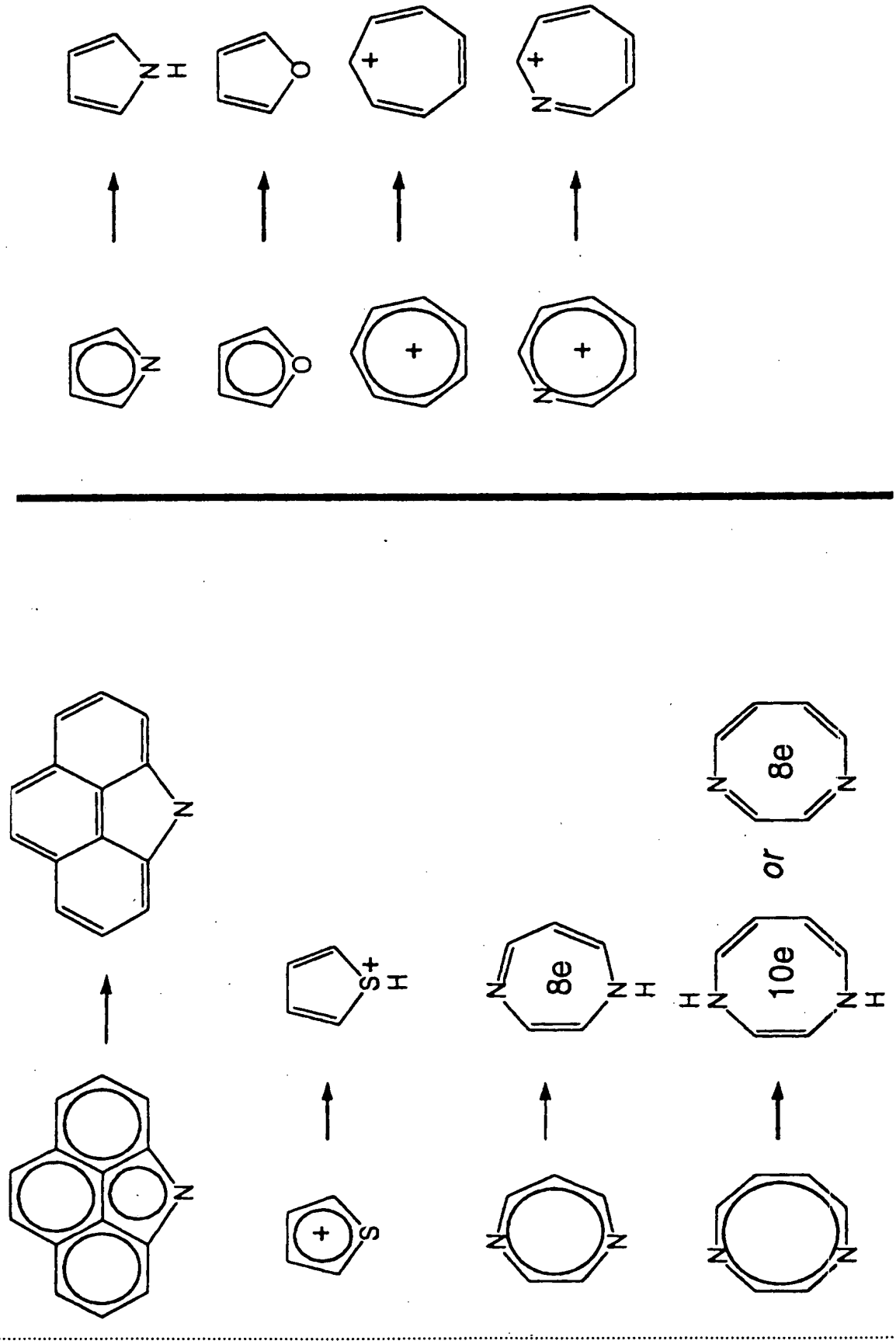

FIG. 17

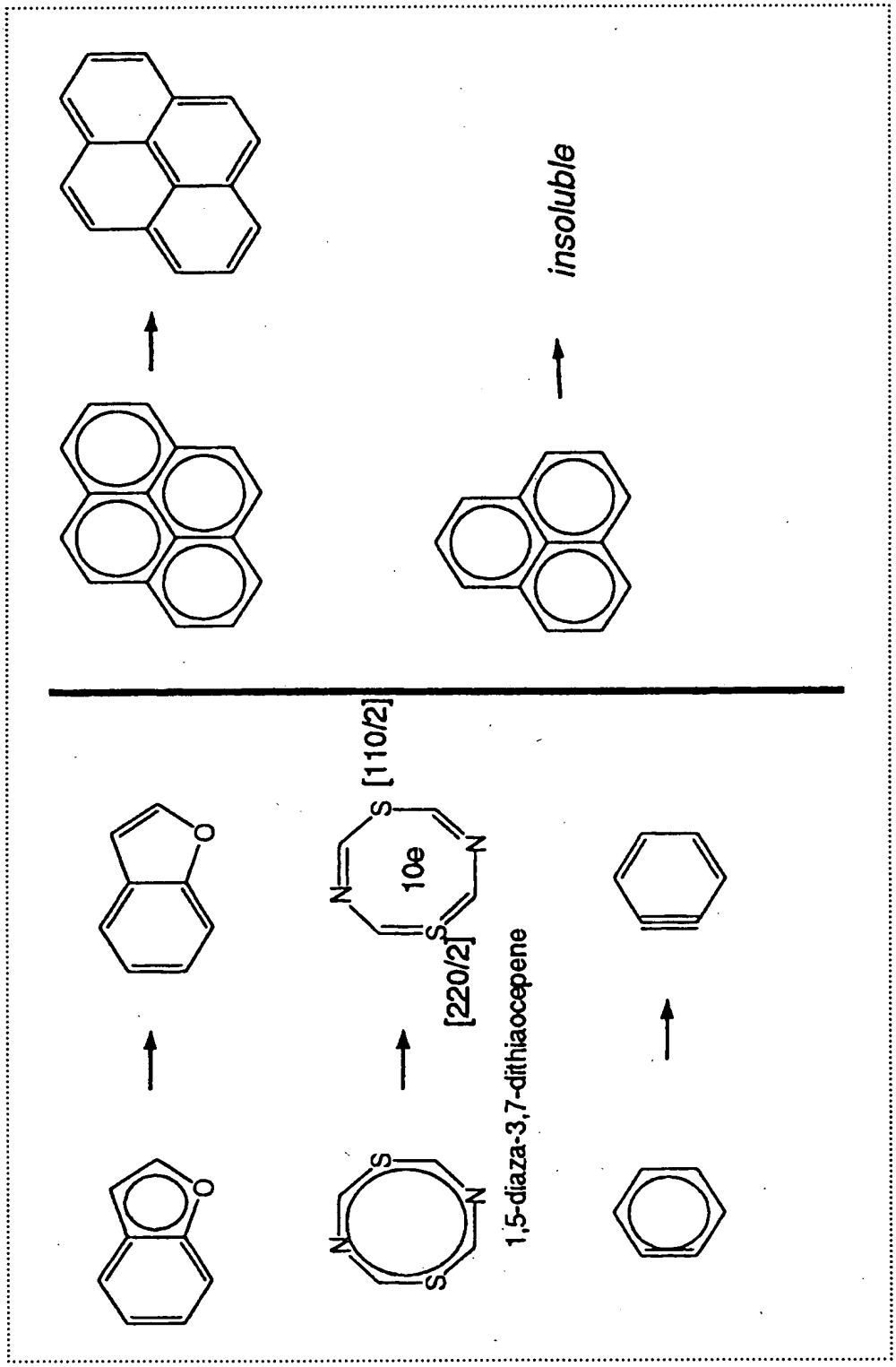

FIG. 18

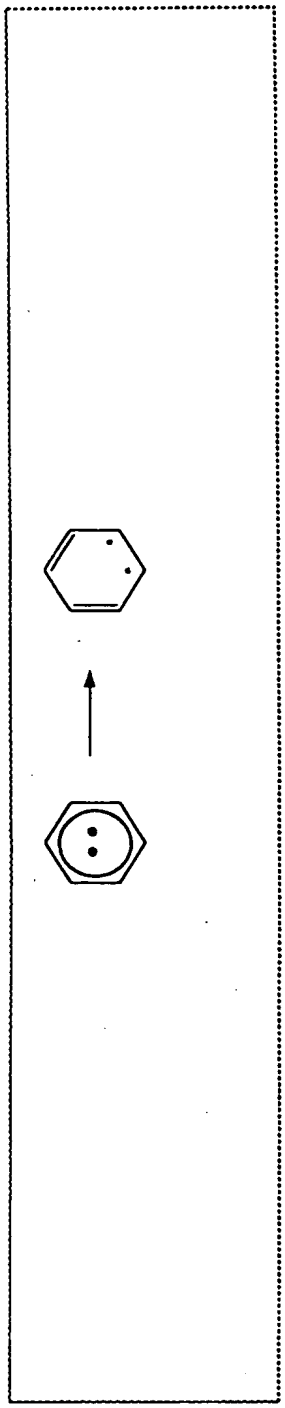

FIG. 19

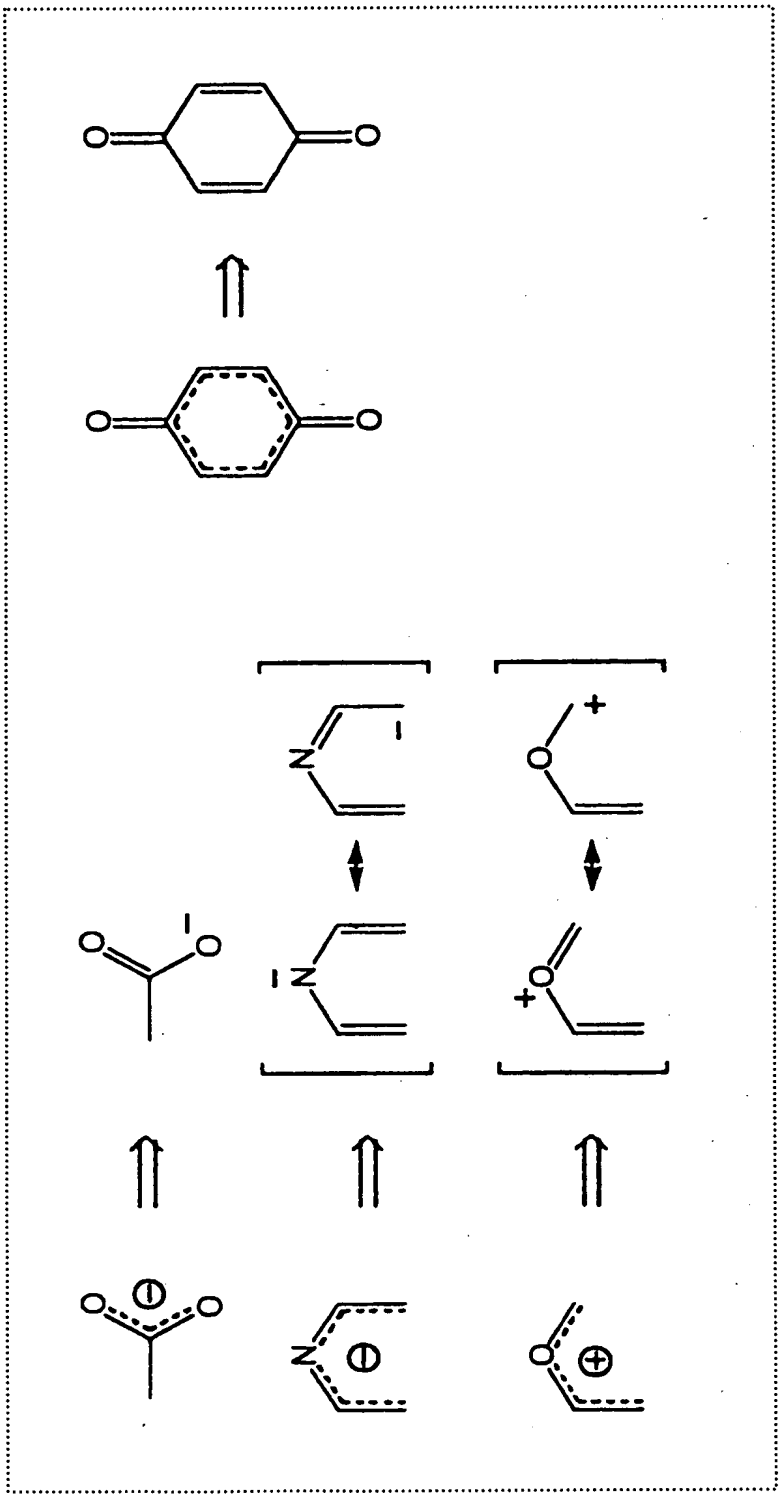

FIG. 20

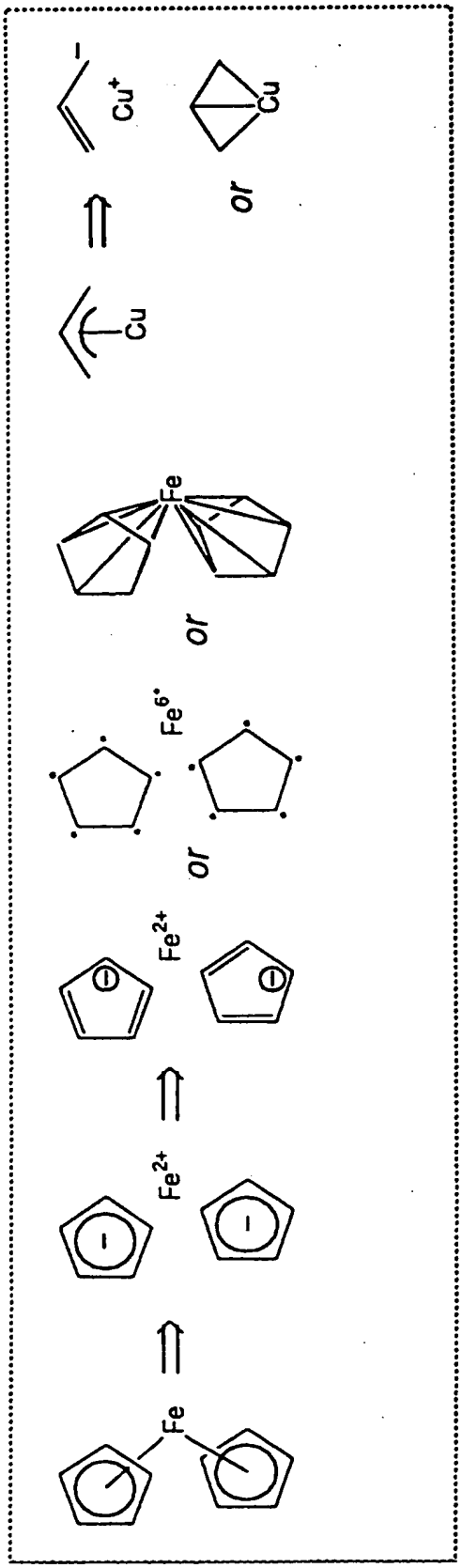

FIG. 21

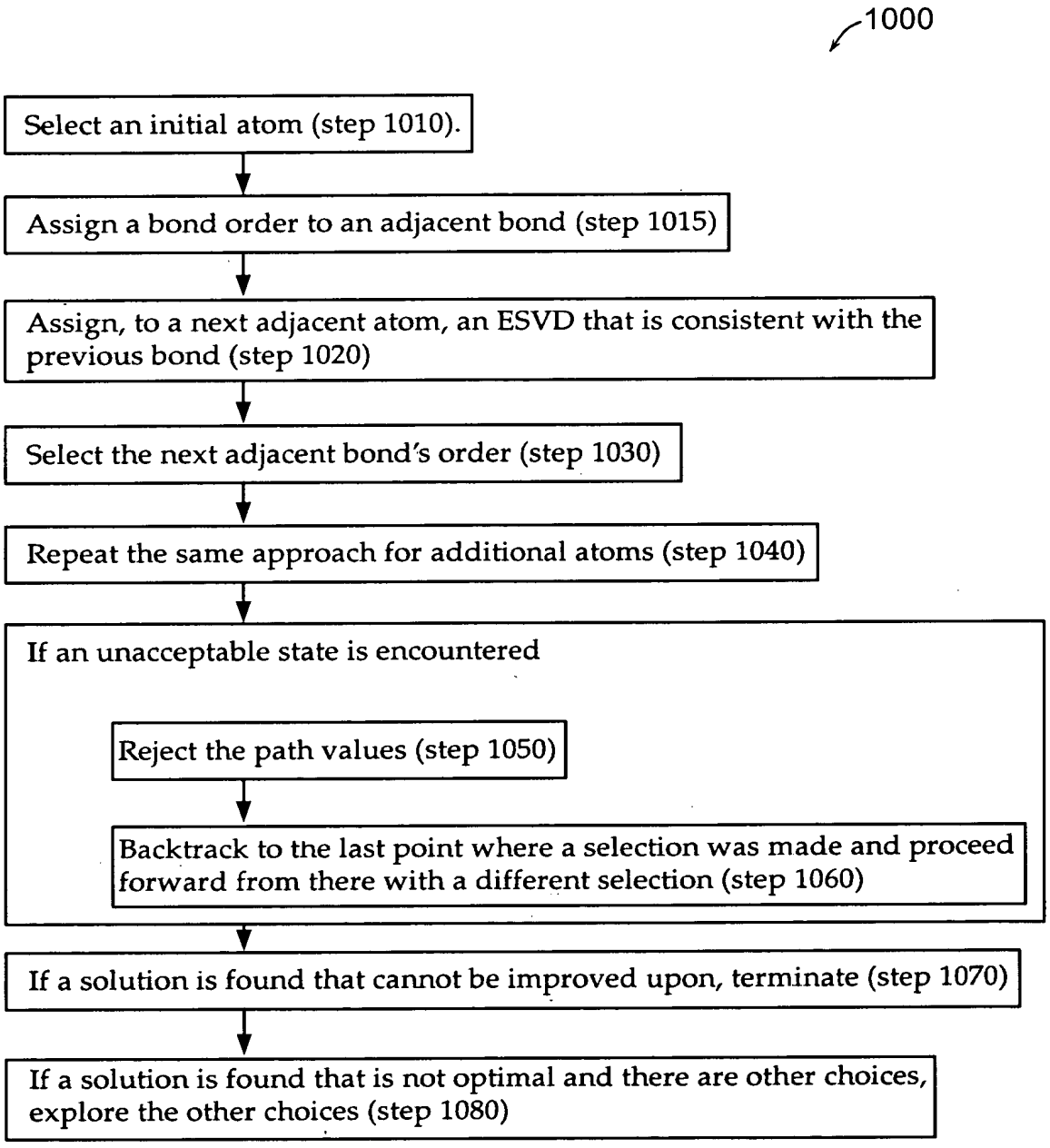

FIG. 22

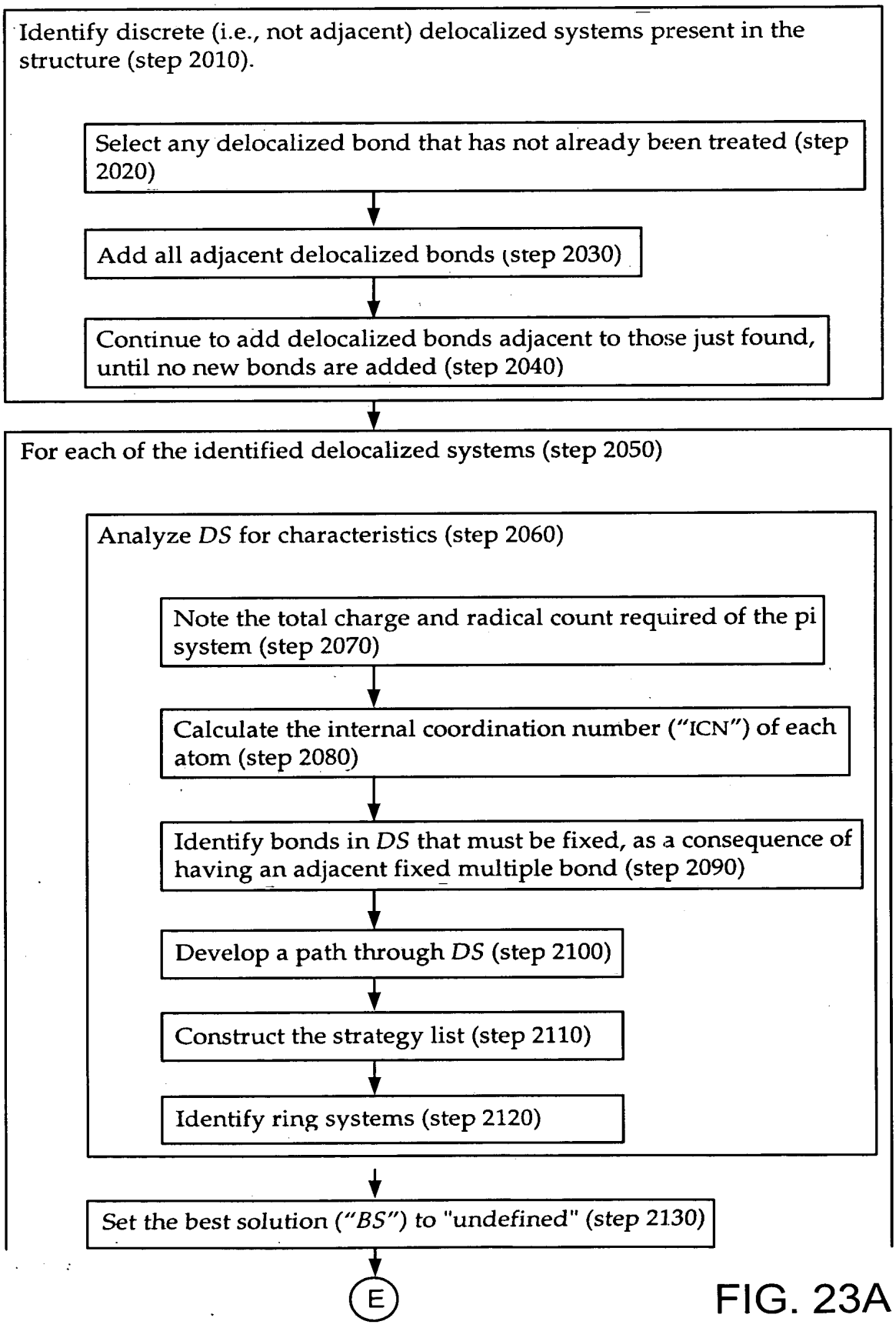

FIG. 23A

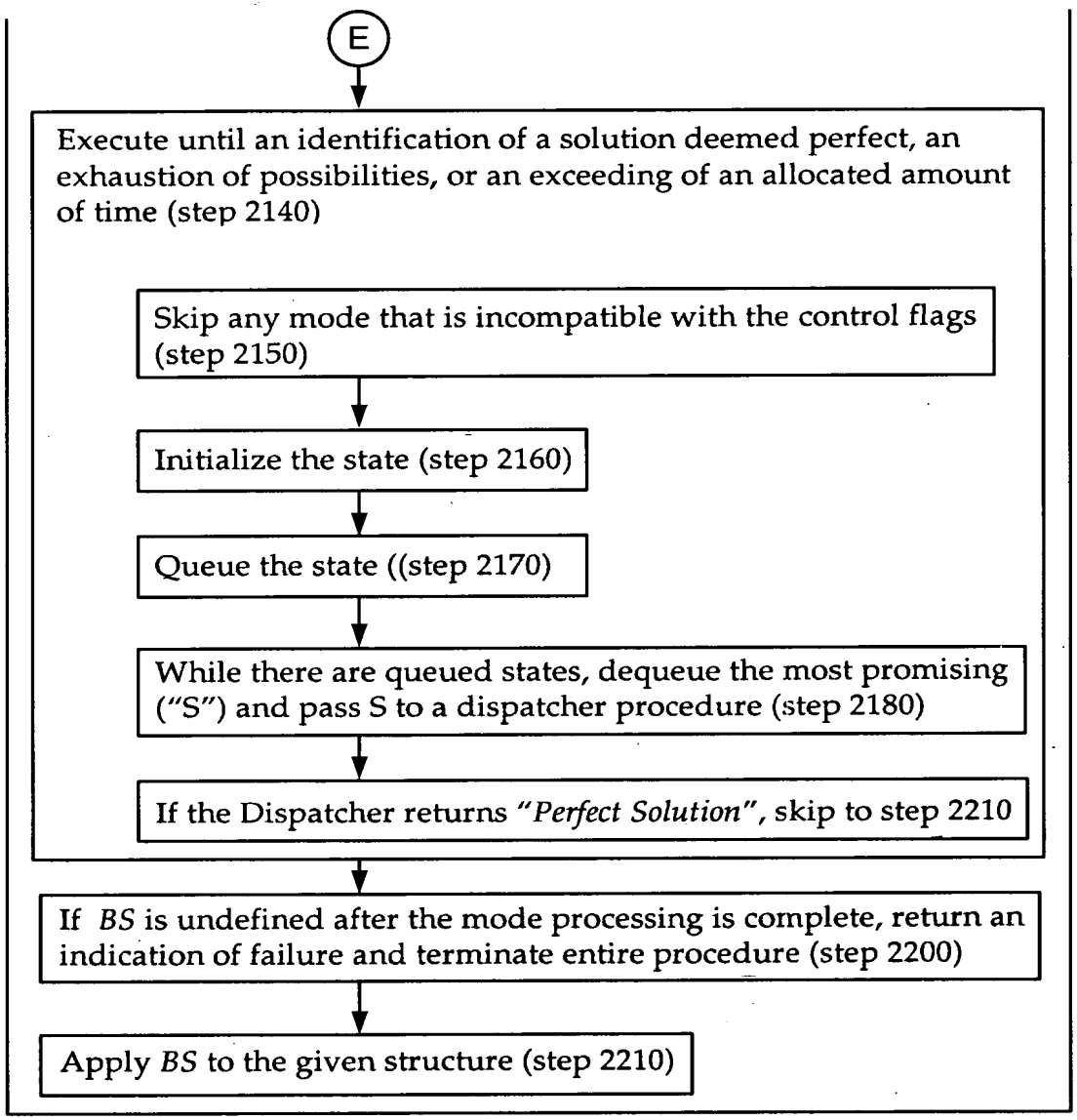

FIG. 23B

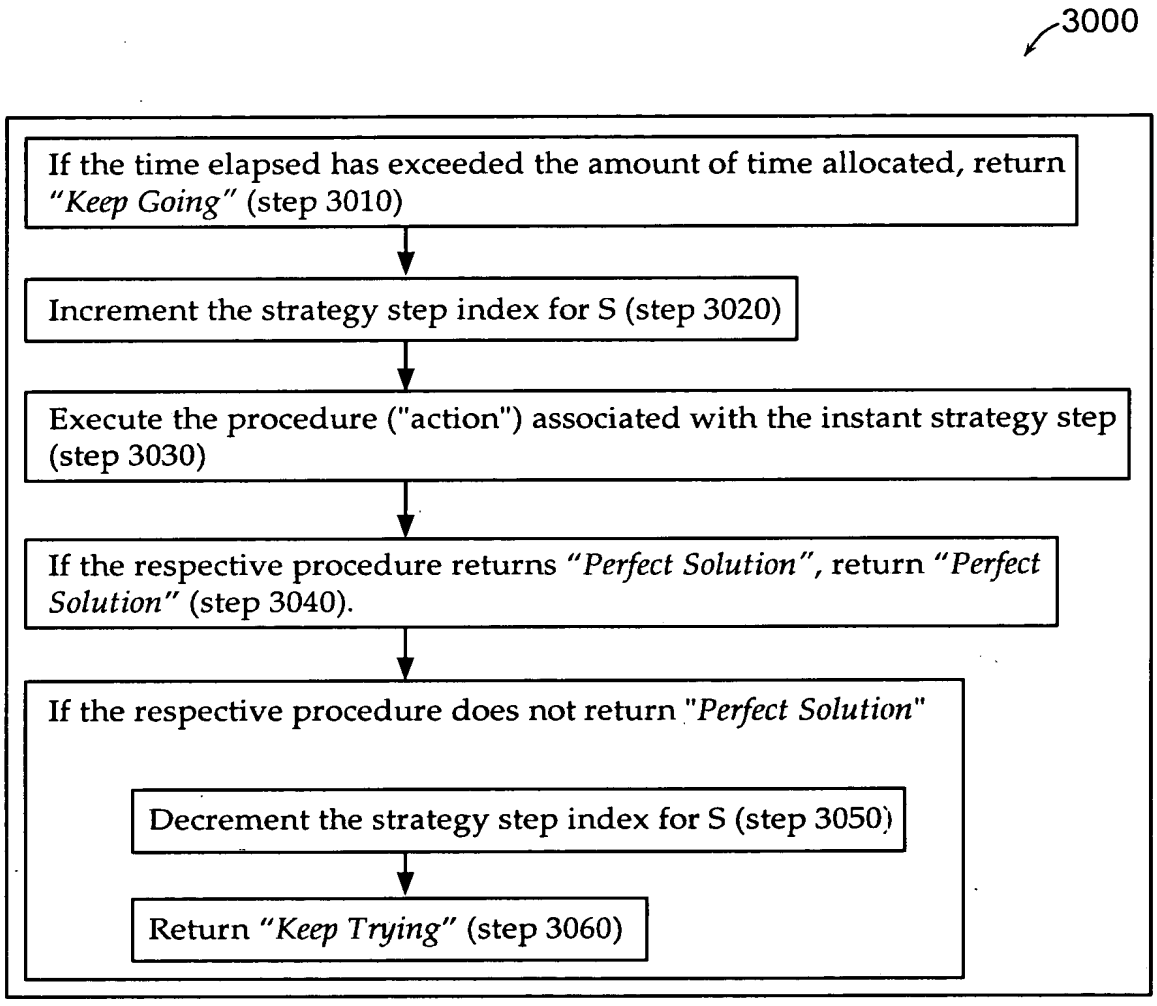

FIG. 24

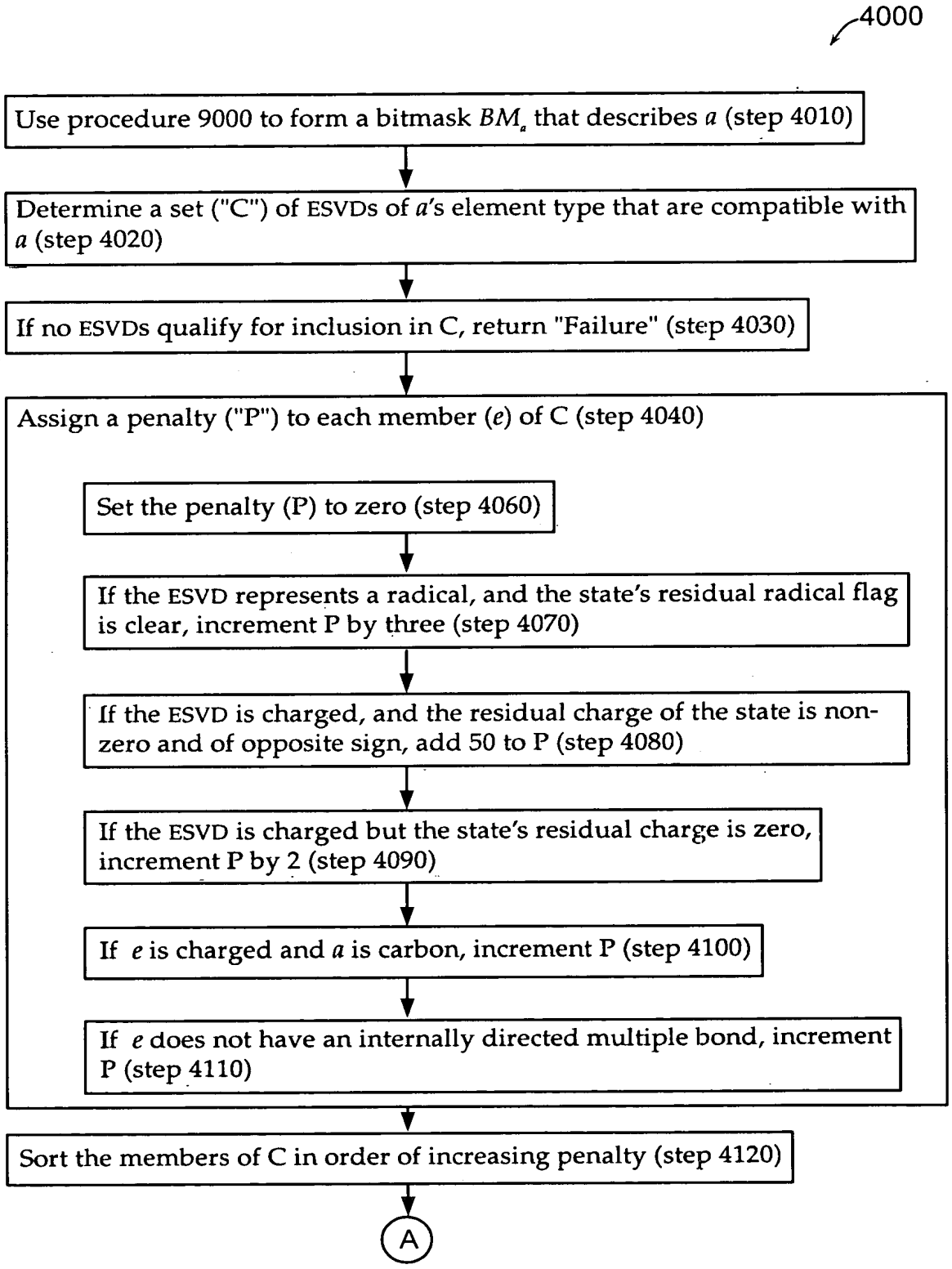

FIG. 25A

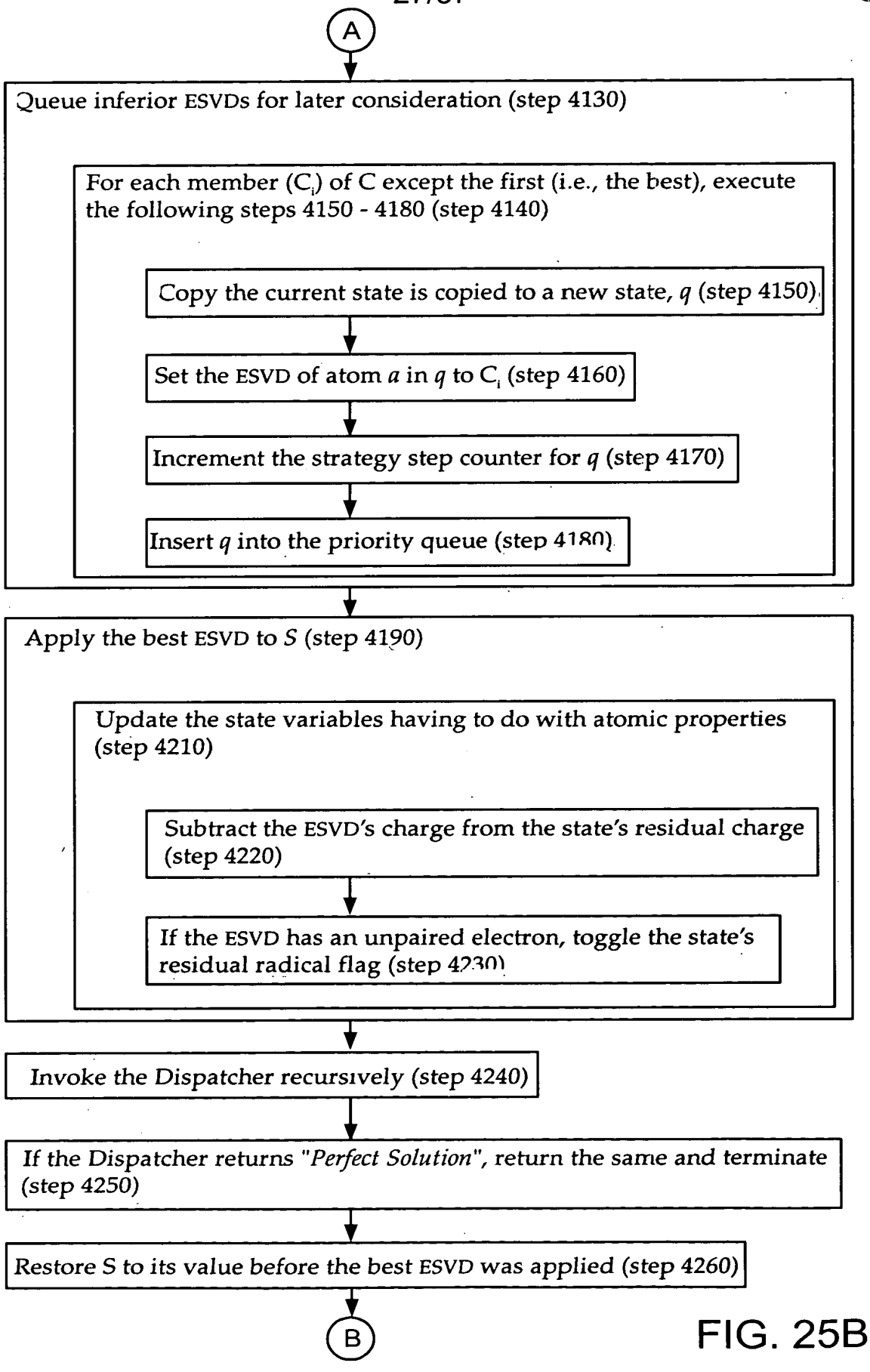

FIG. 25B

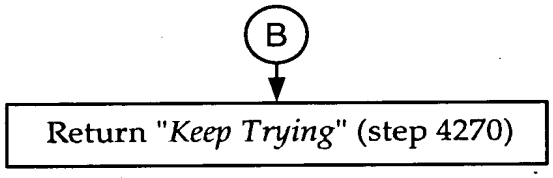

FIG. 25C

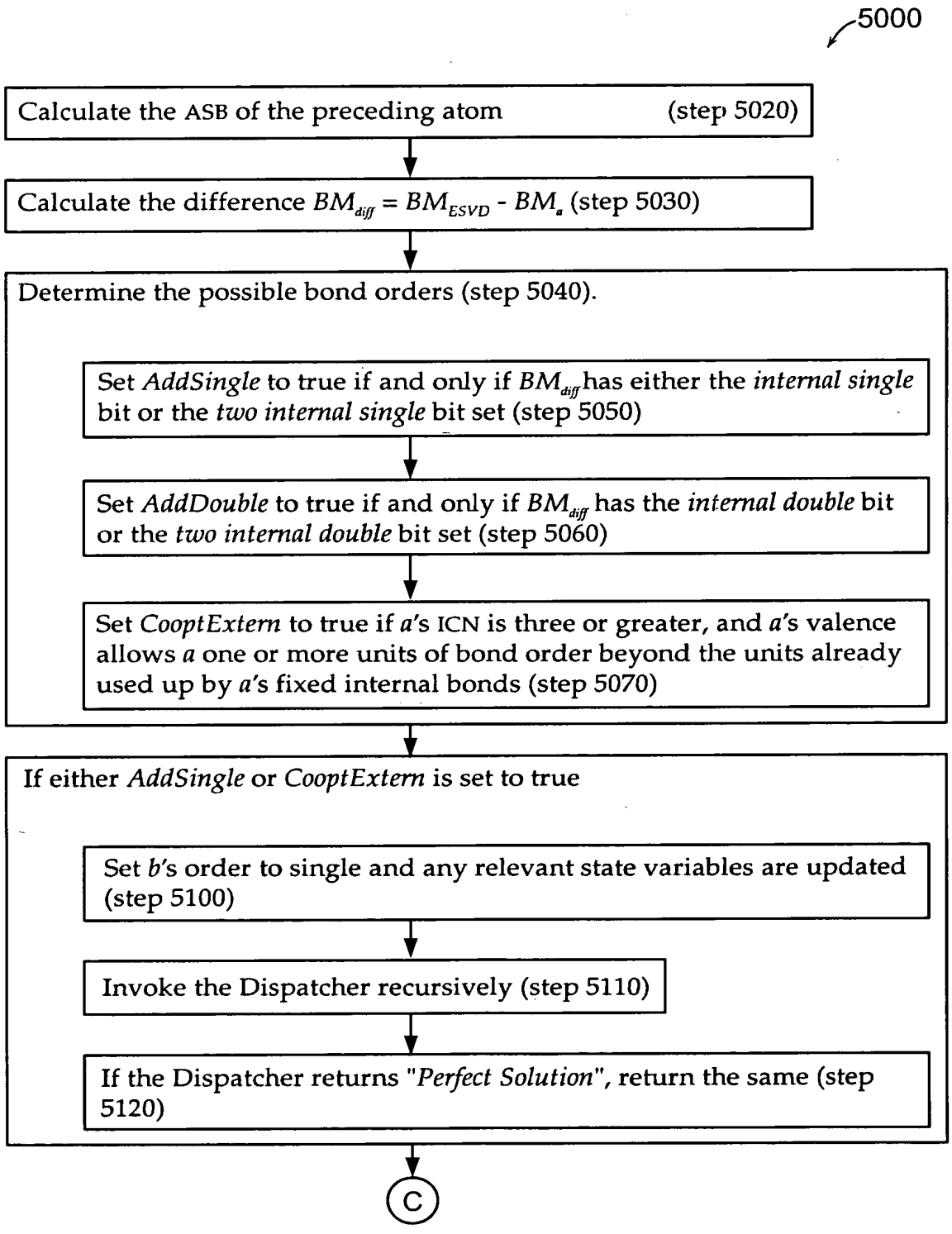

FIG. 26A

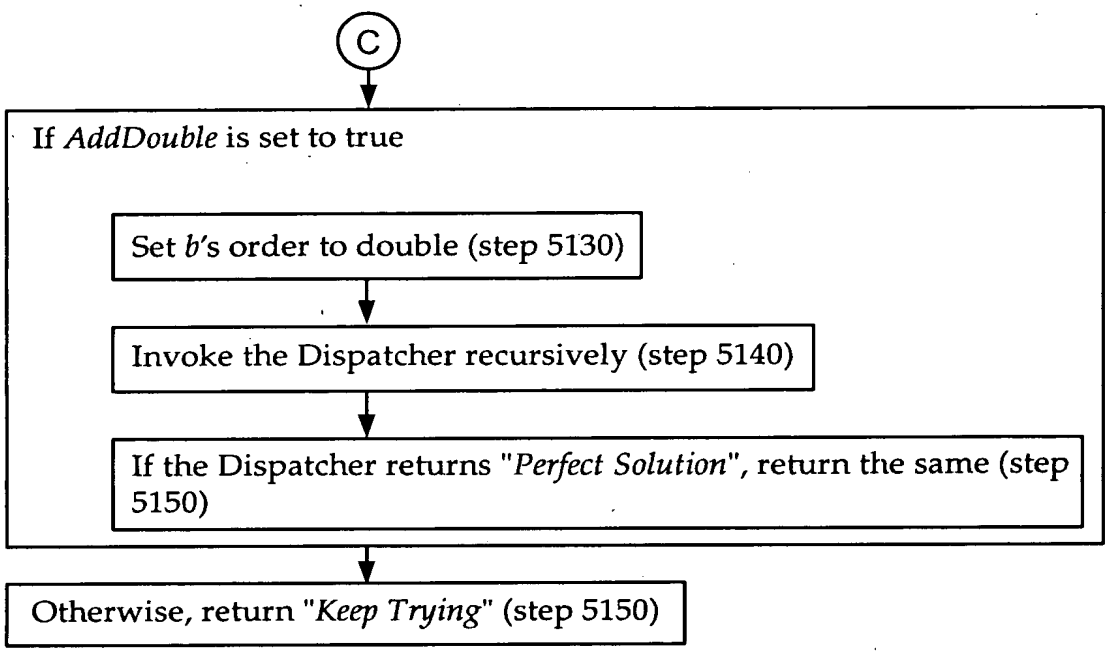

FIG. 26B

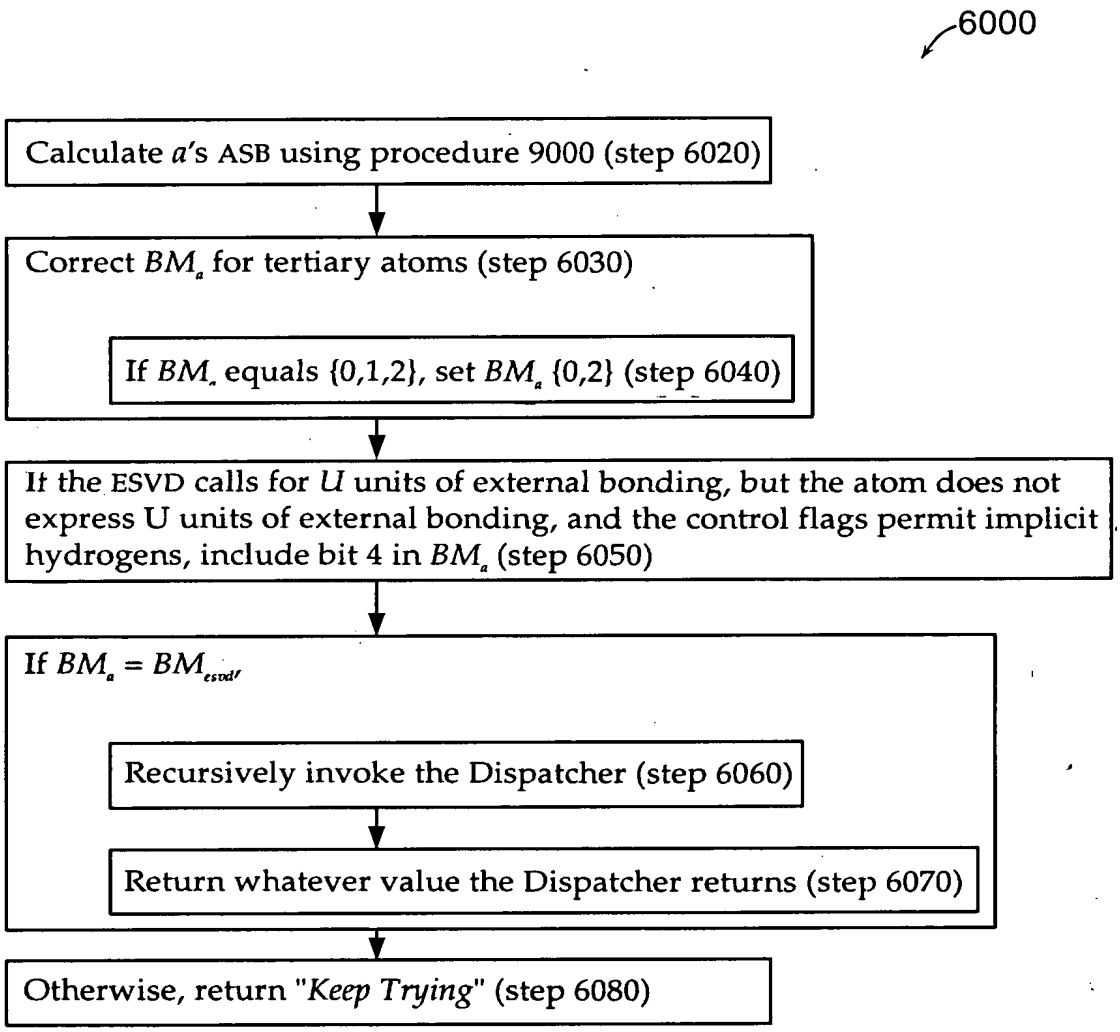

FIG. 27

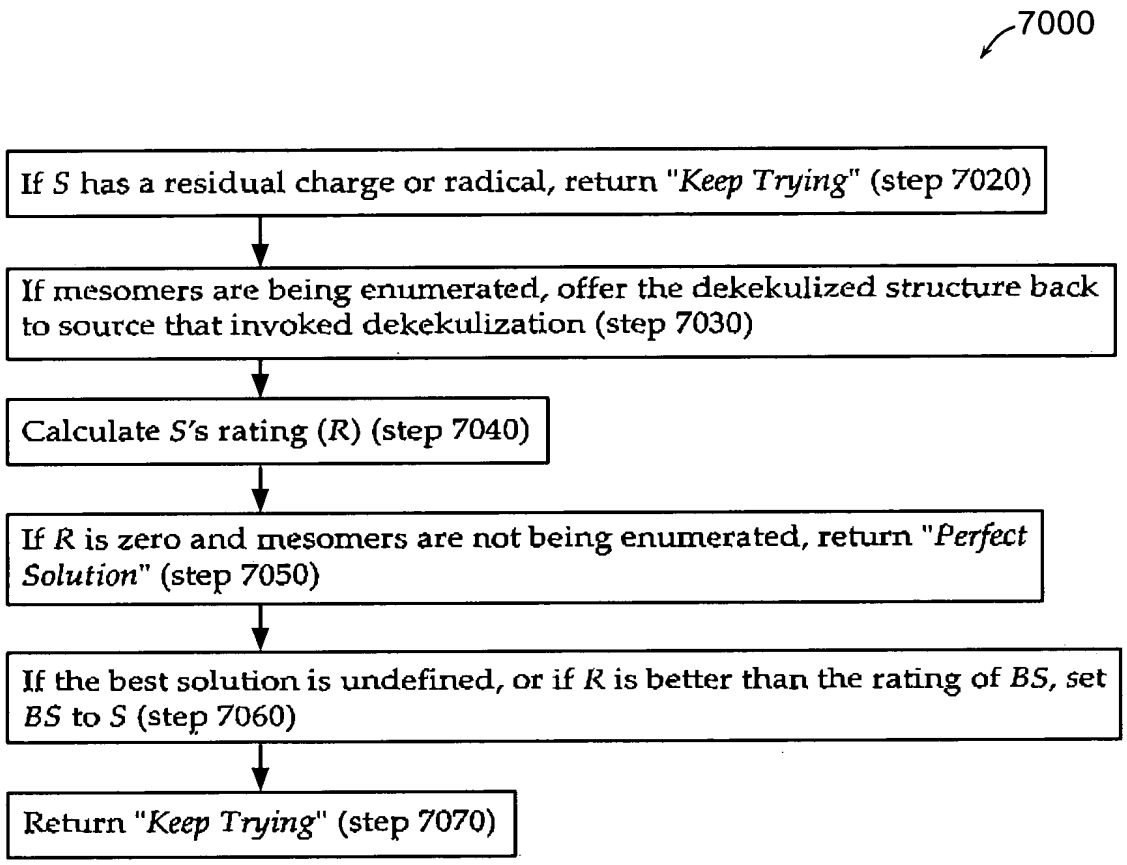

FIG. 28

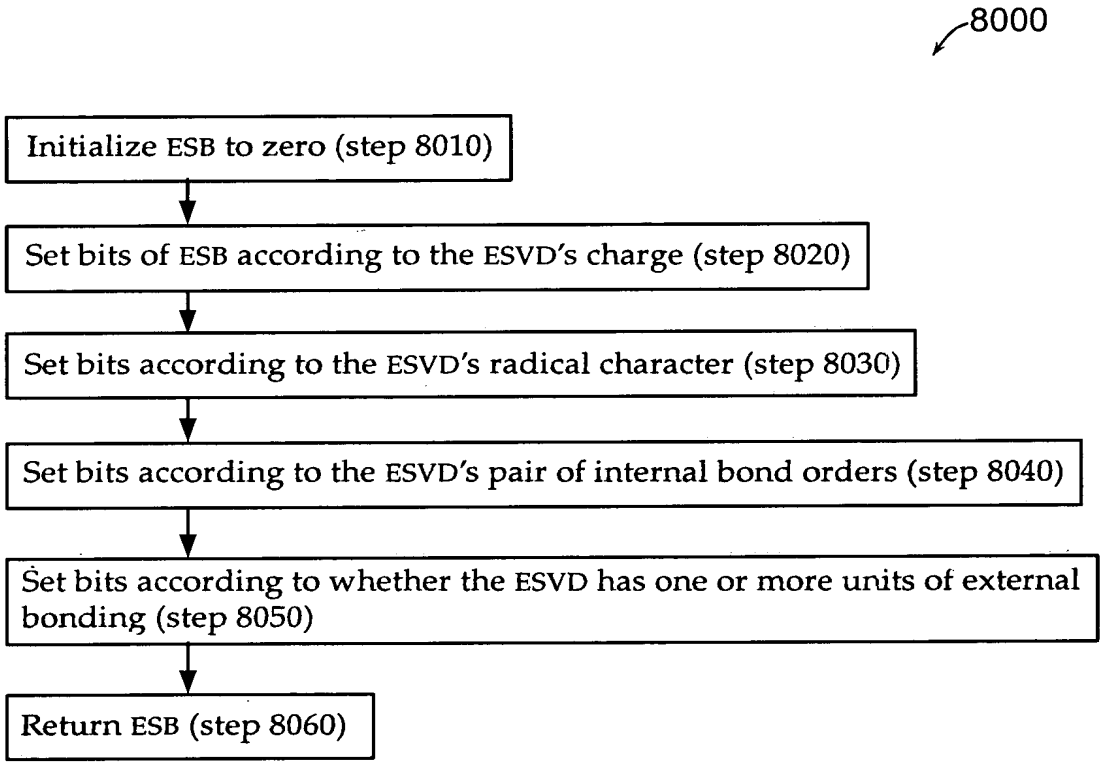

FIG. 29

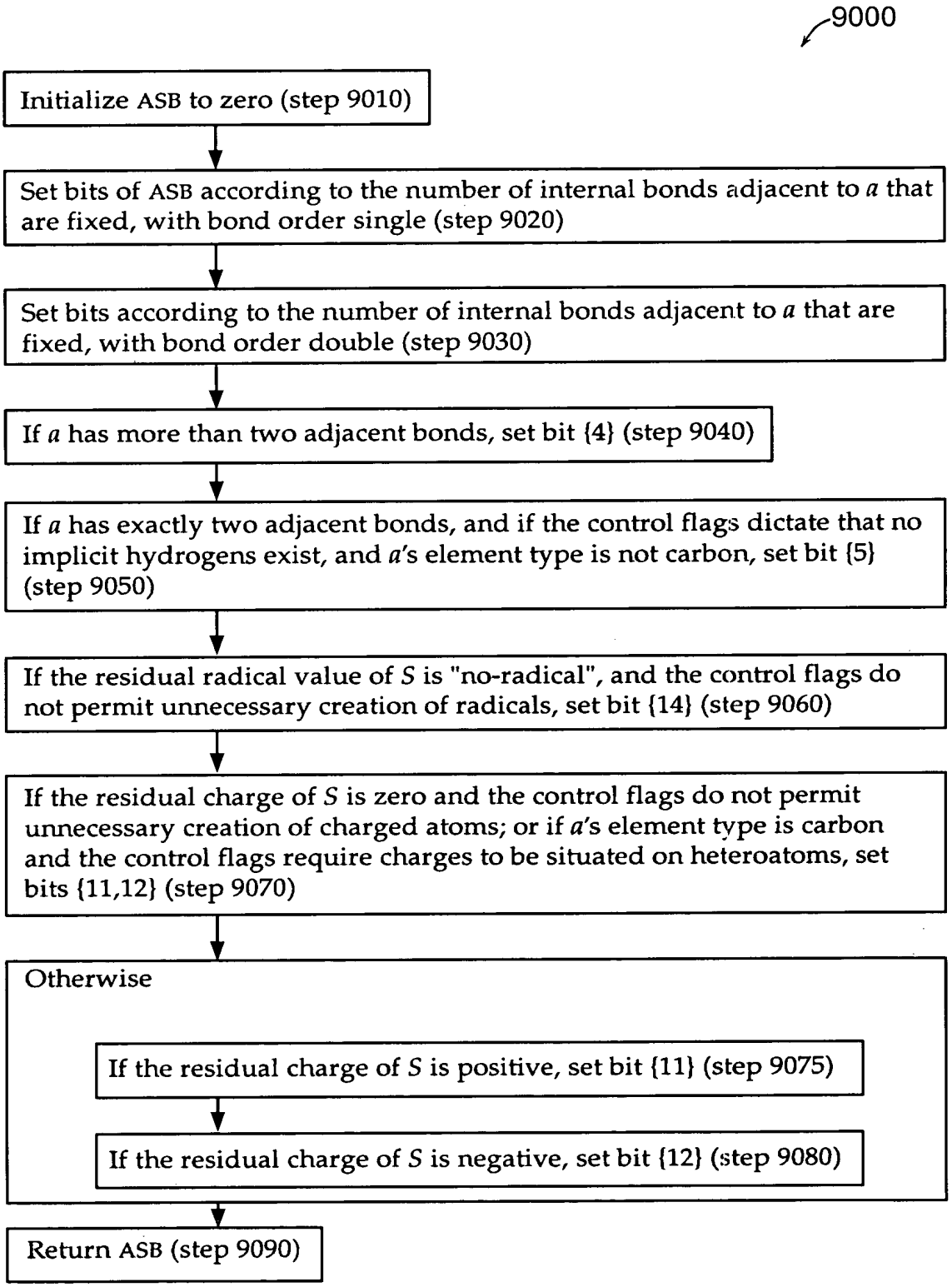

FIG. 30

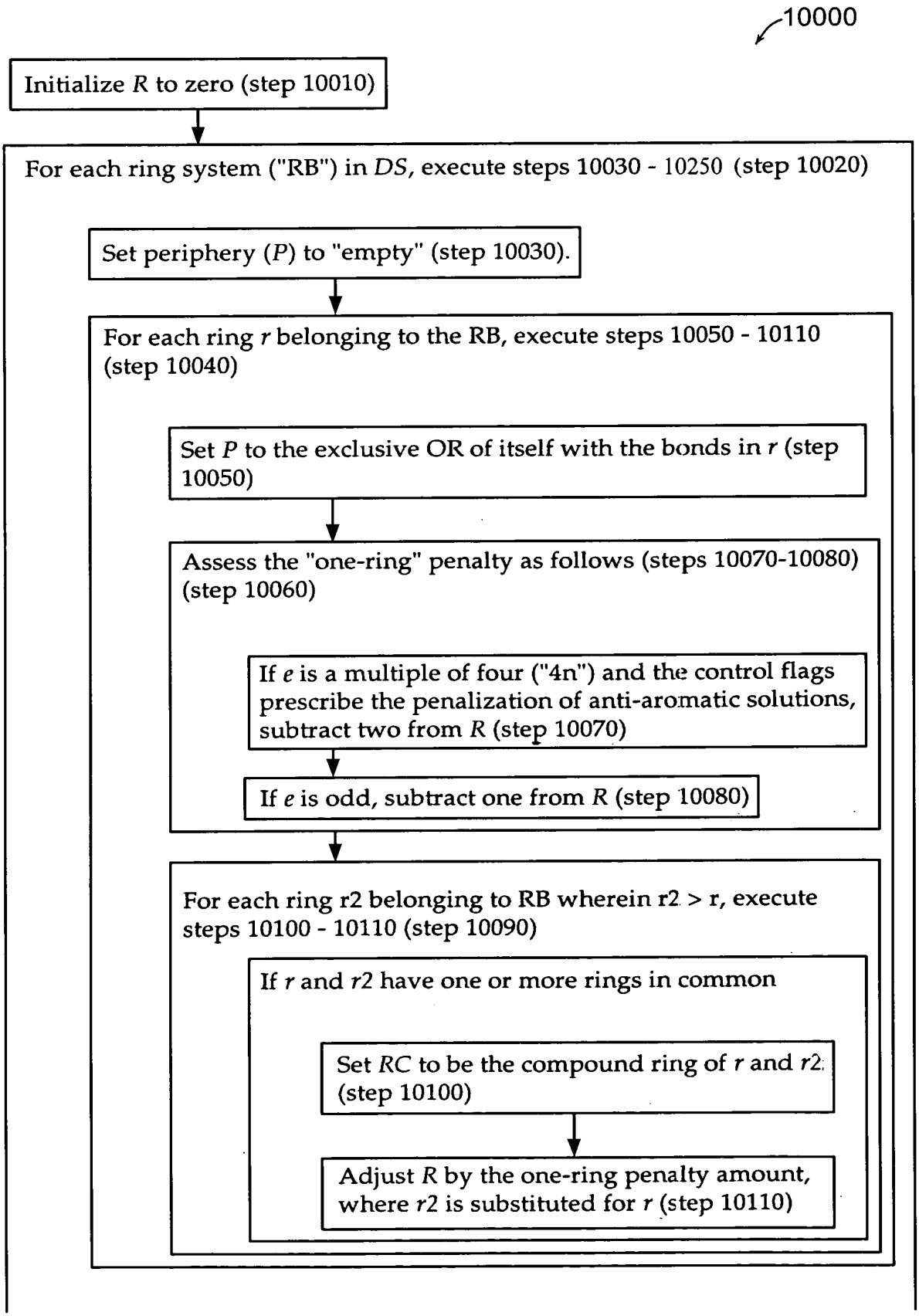

FIG. 31A

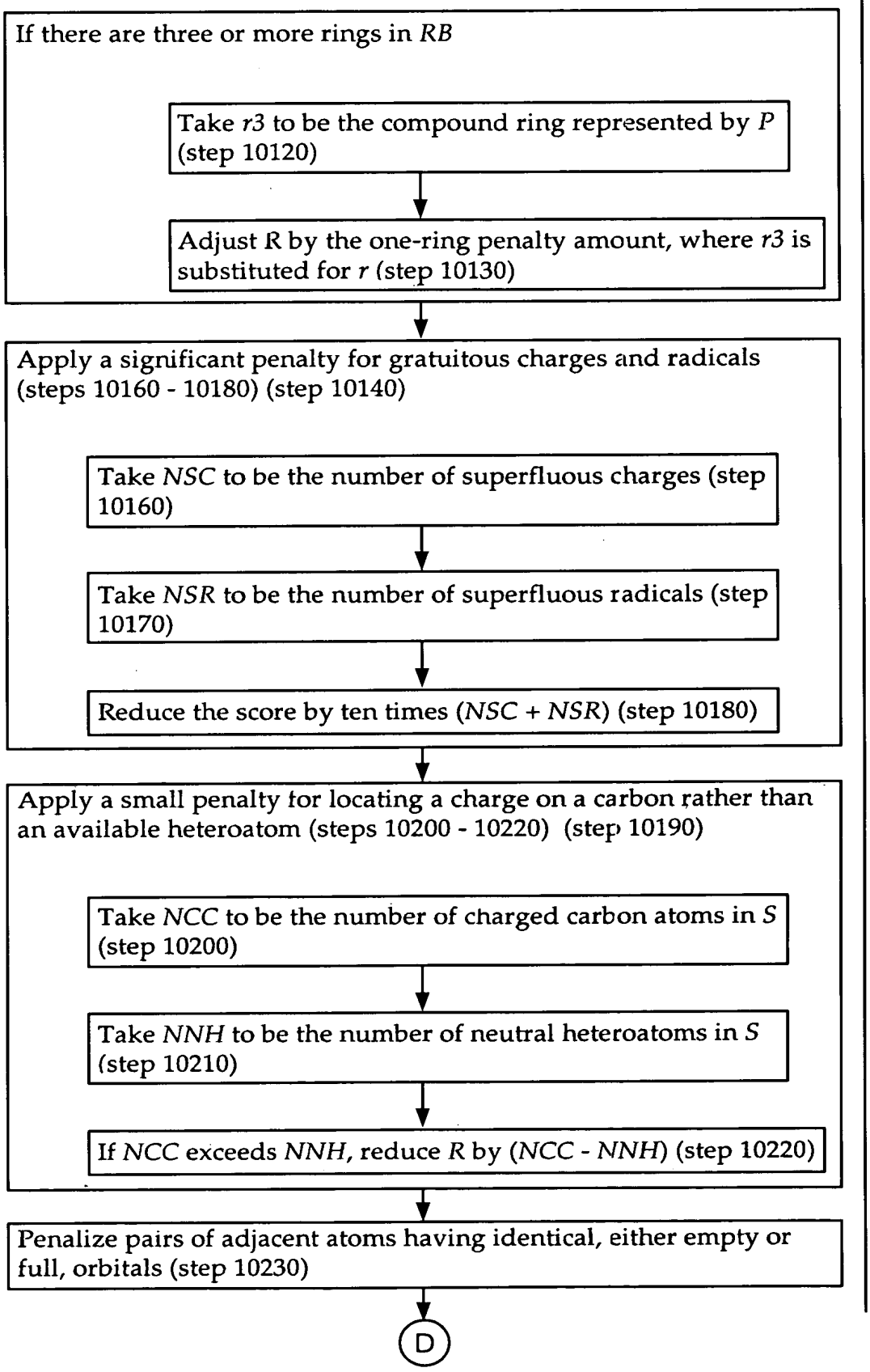

FIG. 31B

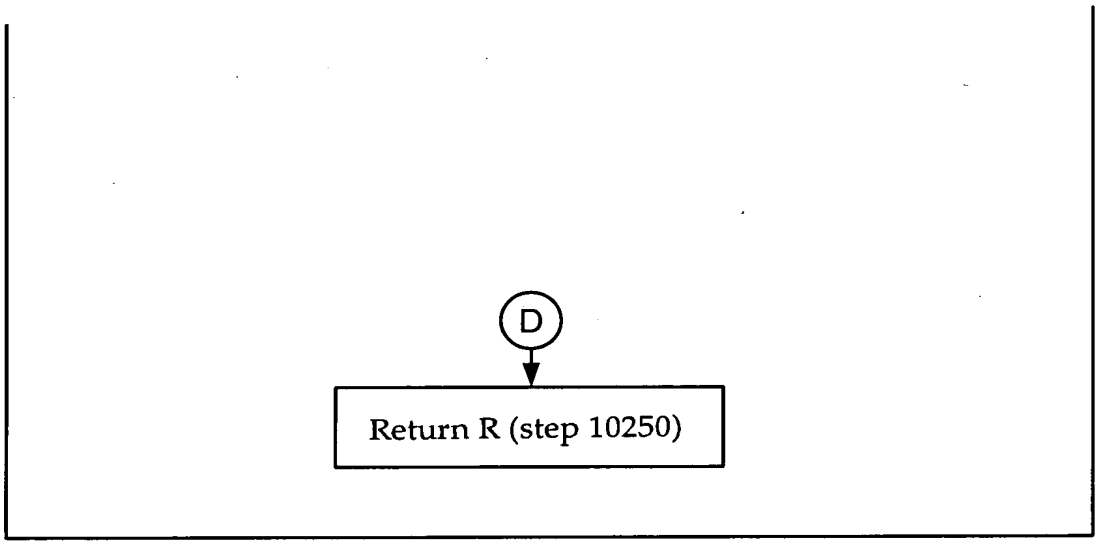

FIG. 31C